



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 06:00 AM GMT

PDB ID : 3A13
Title : Crystal structure of Type III Rubisco SP4 mutant complexed with 2-CABP and activated with Ca
Authors : Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on : 2009-03-25
Resolution : 2.34 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

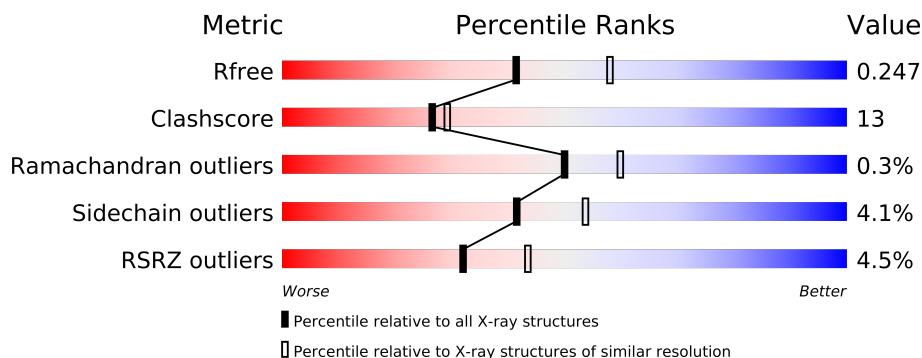
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4049 (2.38-2.30)
Clashscore	79885	1094 (2.36-2.32)
Ramachandran outliers	78287	1080 (2.36-2.32)
Sidechain outliers	78261	1081 (2.36-2.32)
RSRZ outliers	66119	4050 (2.38-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	
1	F	444	
1	G	444	
1	H	444	
1	I	444	
1	J	444	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	C	445	-	X
2	MG	H	445	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36193 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3408	2186	586	626	10			
1	B	437	Total	C	N	O	S	0	0	0
			3412	2187	586	629	10			
1	C	437	Total	C	N	O	S	0	0	0
			3399	2181	584	624	10			
1	D	437	Total	C	N	O	S	0	0	0
			3392	2170	584	628	10			
1	E	432	Total	C	N	O	S	0	0	0
			3379	2163	581	625	10			
1	F	437	Total	C	N	O	S	0	0	0
			3405	2184	586	625	10			
1	G	437	Total	C	N	O	S	0	0	0
			3413	2190	585	628	10			
1	H	438	Total	C	N	O	S	0	0	0
			3412	2189	588	625	10			
1	I	437	Total	C	N	O	S	0	0	0
			3423	2195	587	631	10			
1	J	434	Total	C	N	O	S	0	0	0
			3379	2161	583	625	10			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	GLU	GLY	ENGINEERED	UNP O93627
A	327	ARG	LYS	ENGINEERED	UNP O93627
A	328	ASP	TRP	ENGINEERED	UNP O93627
A	329	ILE	ASP	ENGINEERED	UNP O93627
A	330	THR	VAL	ENGINEERED	UNP O93627
B	326	GLU	GLY	ENGINEERED	UNP O93627
B	327	ARG	LYS	ENGINEERED	UNP O93627
B	328	ASP	TRP	ENGINEERED	UNP O93627
B	329	ILE	ASP	ENGINEERED	UNP O93627

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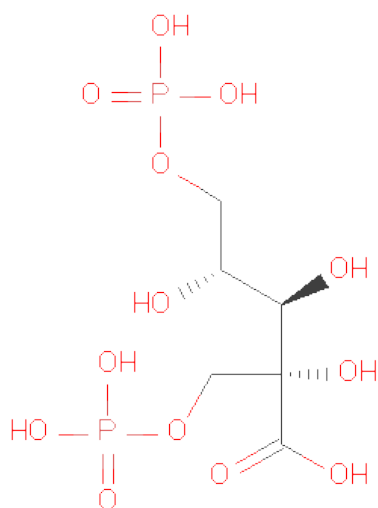
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Chain	Residue	Modelled	Actual	Comment	Reference
B	330	THR	VAL	ENGINEERED	UNP O93627
C	326	GLU	GLY	ENGINEERED	UNP O93627
C	327	ARG	LYS	ENGINEERED	UNP O93627
C	328	ASP	TRP	ENGINEERED	UNP O93627
C	329	ILE	ASP	ENGINEERED	UNP O93627
C	330	THR	VAL	ENGINEERED	UNP O93627
D	326	GLU	GLY	ENGINEERED	UNP O93627
D	327	ARG	LYS	ENGINEERED	UNP O93627
D	328	ASP	TRP	ENGINEERED	UNP O93627
D	329	ILE	ASP	ENGINEERED	UNP O93627
D	330	THR	VAL	ENGINEERED	UNP O93627
E	326	GLU	GLY	ENGINEERED	UNP O93627
E	327	ARG	LYS	ENGINEERED	UNP O93627
E	328	ASP	TRP	ENGINEERED	UNP O93627
E	329	ILE	ASP	ENGINEERED	UNP O93627
E	330	THR	VAL	ENGINEERED	UNP O93627
F	326	GLU	GLY	ENGINEERED	UNP O93627
F	327	ARG	LYS	ENGINEERED	UNP O93627
F	328	ASP	TRP	ENGINEERED	UNP O93627
F	329	ILE	ASP	ENGINEERED	UNP O93627
F	330	THR	VAL	ENGINEERED	UNP O93627
G	326	GLU	GLY	ENGINEERED	UNP O93627
G	327	ARG	LYS	ENGINEERED	UNP O93627
G	328	ASP	TRP	ENGINEERED	UNP O93627
G	329	ILE	ASP	ENGINEERED	UNP O93627
G	330	THR	VAL	ENGINEERED	UNP O93627
H	326	GLU	GLY	ENGINEERED	UNP O93627
H	327	ARG	LYS	ENGINEERED	UNP O93627
H	328	ASP	TRP	ENGINEERED	UNP O93627
H	329	ILE	ASP	ENGINEERED	UNP O93627
H	330	THR	VAL	ENGINEERED	UNP O93627
I	326	GLU	GLY	ENGINEERED	UNP O93627
I	327	ARG	LYS	ENGINEERED	UNP O93627
I	328	ASP	TRP	ENGINEERED	UNP O93627
I	329	ILE	ASP	ENGINEERED	UNP O93627
I	330	THR	VAL	ENGINEERED	UNP O93627
J	326	GLU	GLY	ENGINEERED	UNP O93627
J	327	ARG	LYS	ENGINEERED	UNP O93627
J	328	ASP	TRP	ENGINEERED	UNP O93627
J	329	ILE	ASP	ENGINEERED	UNP O93627
J	330	THR	VAL	ENGINEERED	UNP O93627

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: C₆H₁₄O₁₃P₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 21 6 13 2	0	0
3	B	1	Total C O P 21 6 13 2	0	0
3	C	1	Total C O P 21 6 13 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	O	P	0	0
			21	6	13	2		
3	E	1	Total	C	O	P	0	0
			21	6	13	2		
3	F	1	Total	C	O	P	0	0
			21	6	13	2		
3	G	1	Total	C	O	P	0	0
			21	6	13	2		
3	H	1	Total	C	O	P	0	0
			21	6	13	2		
3	I	1	Total	C	O	P	0	0
			21	6	13	2		
3	J	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total	O	0	0
			193	193		
5	B	204	Total	O	0	0
			204	204		
5	C	186	Total	O	0	0
			186	186		
5	D	210	Total	O	0	0
			210	210		
5	E	193	Total	O	0	0
			193	193		
5	F	176	Total	O	0	0
			176	176		
5	G	203	Total	O	0	0
			203	203		
5	H	180	Total	O	0	0
			180	180		

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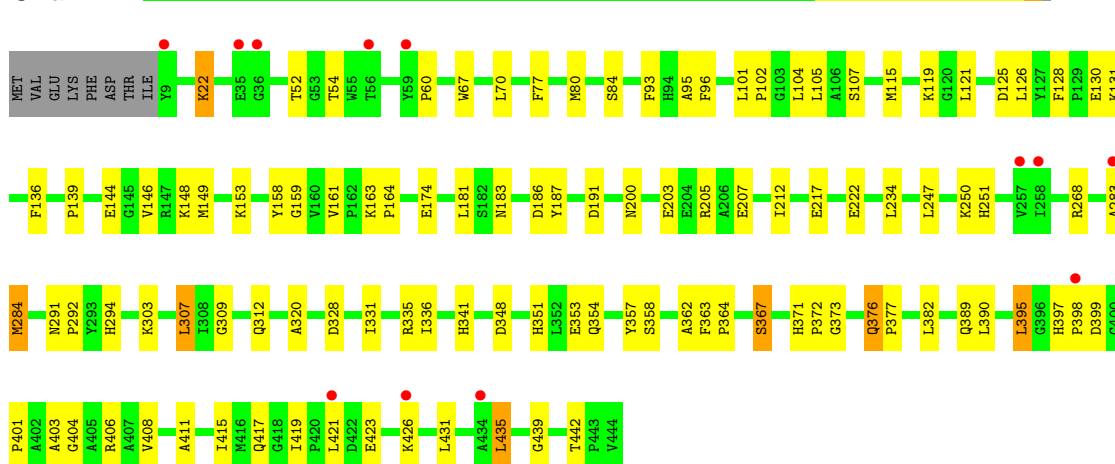
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	212	Total 212	O 212	0	0
5	J	194	Total 194	O 194	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

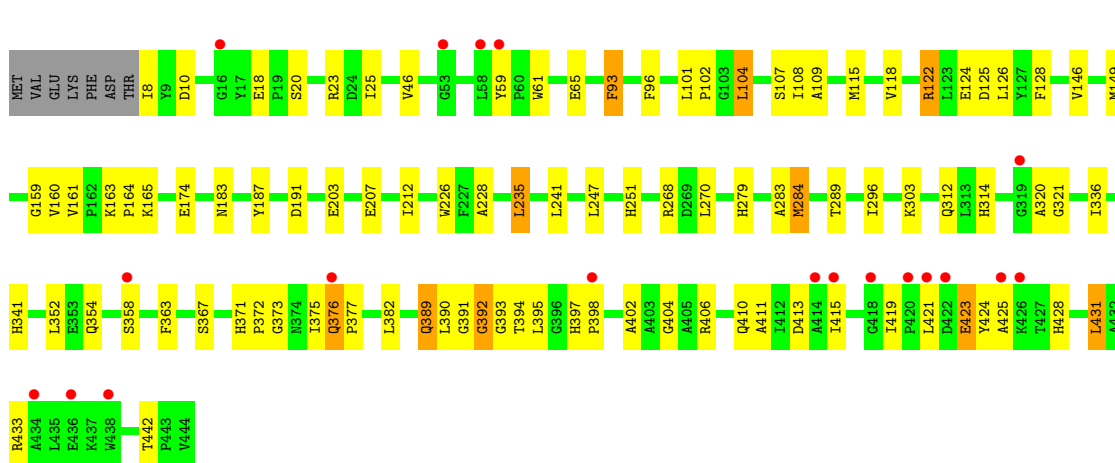
- Molecule 1: Ribulose biphosphate carboxylase

Chain A:



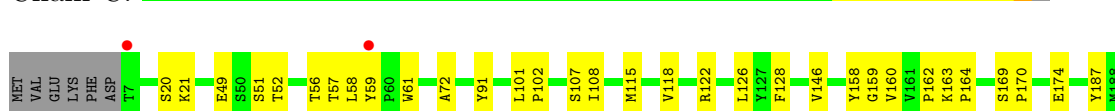
- Molecule 1: Ribulose biphosphate carboxylase

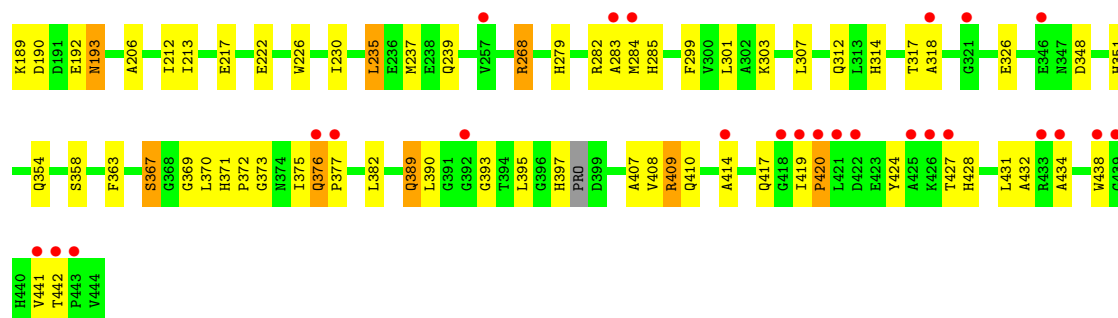
Chain B:



- Molecule 1: Ribulose biphosphate carboxylase

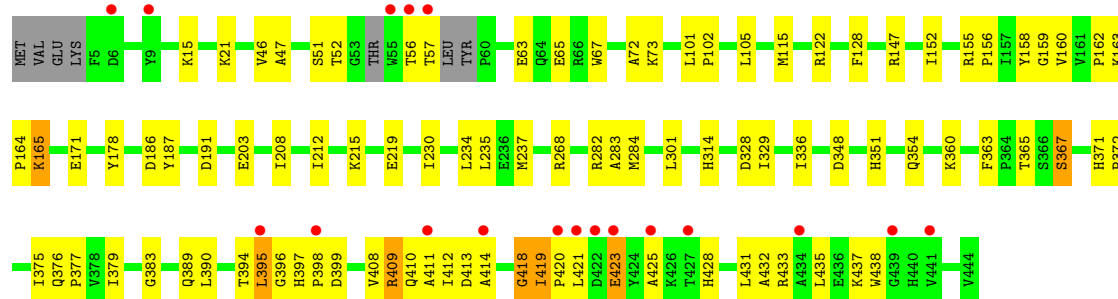
Chain C:





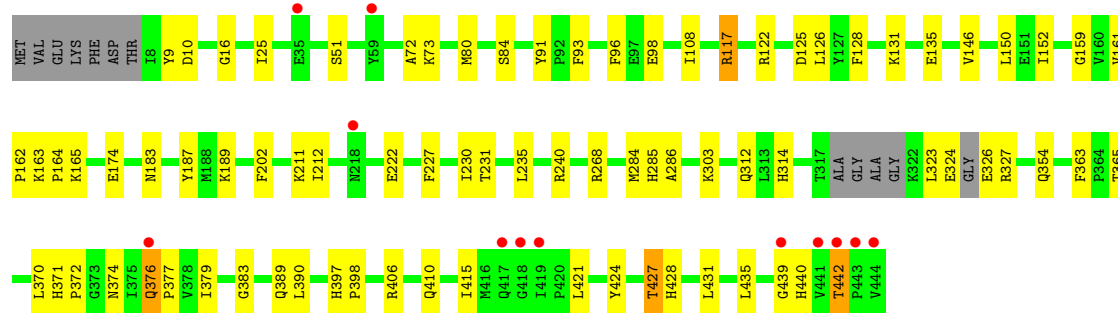
• Molecule 1: Ribulose biphosphate carboxylase

Chain D:



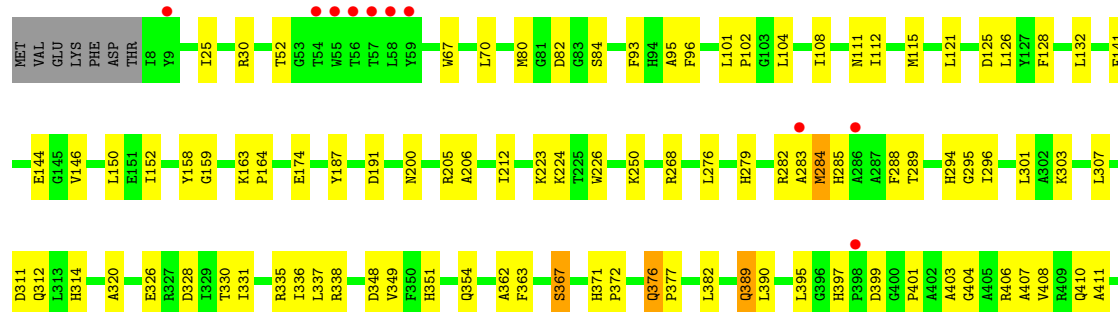
• Molecule 1: Ribulose biphosphate carboxylase

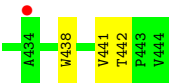
Chain E:



• Molecule 1: Ribulose biphosphate carboxylase

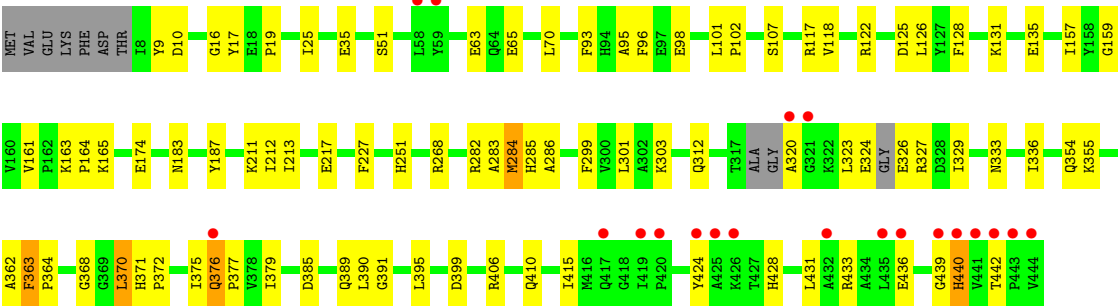
Chain F:





● Molecule 1: Ribulose biphosphate carboxylase

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.68Å 247.09Å 144.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.22 – 2.34 42.22 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.22-2.34) 99.4 (42.22-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.205 , 0.250 0.206 , 0.247	Depositor DCC
R_{free} test set	13142 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	4 of 261352 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36193	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.31 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.5974e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CAP, MG, KCX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/3482	0.51	0/4722
1	B	0.37	0/3486	0.52	0/4729
1	C	0.35	0/3472	0.50	0/4711
1	D	0.38	0/3463	0.51	0/4695
1	E	0.37	0/3451	0.51	0/4680
1	F	0.35	0/3479	0.50	0/4719
1	G	0.37	0/3488	0.51	0/4732
1	H	0.37	0/3486	0.51	0/4729
1	I	0.39	0/3495	0.53	0/4735
1	J	0.38	0/3451	0.51	0/4679
All	All	0.37	0/34753	0.51	0/47131

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3408	0	3311	86	0
1	B	3412	0	3307	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3399	0	3284	89	0
1	D	3392	0	3267	91	0
1	E	3379	0	3253	74	0
1	F	3405	0	3301	73	0
1	G	3413	0	3303	86	0
1	H	3412	0	3315	95	0
1	I	3423	0	3330	83	0
1	J	3379	0	3235	81	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
3	A	21	0	7	1	0
3	B	21	0	7	1	0
3	C	21	0	7	3	0
3	D	21	0	7	0	0
3	E	21	0	9	1	0
3	F	21	0	8	2	0
3	G	21	0	7	1	0
3	H	21	0	8	2	0
3	I	21	0	7	0	0
3	J	21	0	9	1	0
4	E	1	0	0	0	0
4	J	1	0	0	0	0
5	A	193	0	0	15	0
5	B	204	0	0	14	0
5	C	186	0	0	9	0
5	D	210	0	0	16	0
5	E	193	0	0	12	0
5	F	176	0	0	9	0
5	G	203	0	0	14	0
5	H	180	0	0	6	0
5	I	212	0	0	14	0
5	J	194	0	0	10	0
All	All	36193	0	32982	885	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 885 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:326:GLU:HG2	5:F:602:HOH:O	1.45	1.16
1:J:174:GLU:HG3	1:J:212:ILE:HD11	1.29	1.13
1:J:391:GLY:O	1:J:395:LEU:HD12	1.49	1.12
1:E:174:GLU:HG3	1:E:212:ILE:HD11	1.28	1.11
1:I:429:LYS:H	1:I:429:LYS:HD3	0.98	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/444 (98%)	417 (96%)	13 (3%)	3 (1%)	30	33
1	B	434/444 (98%)	413 (95%)	19 (4%)	2 (0%)	38	44
1	C	432/444 (97%)	408 (94%)	23 (5%)	1 (0%)	56	67
1	D	430/444 (97%)	401 (93%)	26 (6%)	3 (1%)	30	33
1	E	425/444 (96%)	410 (96%)	14 (3%)	1 (0%)	56	67
1	F	434/444 (98%)	409 (94%)	23 (5%)	2 (0%)	38	44
1	G	434/444 (98%)	411 (95%)	23 (5%)	0	100	100
1	H	435/444 (98%)	415 (95%)	20 (5%)	0	100	100
1	I	430/444 (97%)	411 (96%)	18 (4%)	1 (0%)	56	67
1	J	427/444 (96%)	407 (95%)	19 (4%)	1 (0%)	56	67
All	All	4314/4440 (97%)	4102 (95%)	198 (5%)	14 (0%)	50	60

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	MET
1	E	284	MET
1	F	284	MET
1	F	401	PRO

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Mol	Chain	Res	Type
1	I	284	MET

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/356 (94%)	320 (95%)	16 (5%)	35	45
1	B	336/356 (94%)	320 (95%)	16 (5%)	35	45
1	C	332/356 (93%)	315 (95%)	17 (5%)	33	41
1	D	332/356 (93%)	318 (96%)	14 (4%)	40	52
1	E	333/356 (94%)	322 (97%)	11 (3%)	50	64
1	F	334/356 (94%)	324 (97%)	10 (3%)	53	68
1	G	335/356 (94%)	321 (96%)	14 (4%)	40	52
1	H	335/356 (94%)	326 (97%)	9 (3%)	57	72
1	I	339/356 (95%)	322 (95%)	17 (5%)	34	42
1	J	329/356 (92%)	317 (96%)	12 (4%)	47	60
All	All	3341/3560 (94%)	3205 (96%)	136 (4%)	41	54

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	419	ILE
1	F	301	LEU
1	J	35	GLU
1	E	10	ASP
1	E	268	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	428	HIS
1	F	294	HIS
1	I	351	HIS

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Mol	Chain	Res	Type
1	E	218	ASN
1	E	354	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	A	189	1,2	11,11,12	5.48	2 (18%)	10,12,14	1.54	3 (30%)
1	KCX	B	189	1,2	11,11,12	5.04	1 (9%)	10,12,14	1.78	3 (30%)
1	KCX	C	189	1,2	11,11,12	5.13	2 (18%)	10,12,14	1.64	4 (40%)
1	KCX	D	189	1,2	11,11,12	5.16	2 (18%)	10,12,14	1.97	3 (30%)
1	KCX	E	189	1,4	11,11,12	5.22	2 (18%)	10,12,14	1.81	3 (30%)
1	KCX	F	189	1,2	11,11,12	5.66	2 (18%)	10,12,14	1.97	4 (40%)
1	KCX	G	189	1,2	11,11,12	5.37	3 (27%)	10,12,14	1.23	1 (10%)
1	KCX	H	189	1,2	11,11,12	5.24	2 (18%)	10,12,14	1.56	3 (30%)
1	KCX	I	189	1,2	11,11,12	5.33	2 (18%)	10,12,14	1.77	4 (40%)
1	KCX	J	189	1,4	11,11,12	5.31	2 (18%)	10,12,14	1.95	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	B	189	1,2	-	0/8/10/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	D	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	E	189	1,4	-	0/8/10/12	0/0/0/0
1	KCX	F	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	G	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	H	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	I	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	J	189	1,4	-	0/8/10/12	0/0/0/0

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	189	KCX	O-C	18.42	1.24	1.11
1	A	189	KCX	O-C	17.88	1.23	1.11
1	I	189	KCX	O-C	17.34	1.23	1.11
1	G	189	KCX	O-C	17.28	1.23	1.11
1	J	189	KCX	O-C	17.27	1.23	1.11

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	189	KCX	OQ2-CX-NZ	4.05	121.38	116.33
1	D	189	KCX	OQ2-CX-NZ	3.80	121.06	116.33
1	B	189	KCX	C-CA-N	-3.64	110.20	113.83
1	J	189	KCX	C-CA-N	-3.51	110.32	113.83
1	J	189	KCX	OQ1-CX-NZ	-3.50	119.11	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CAP	A	446	2	20,20,20	0.78	0	31,31,31	1.04	2 (6%)
3	CAP	B	446	2	20,20,20	0.77	0	31,31,31	1.11	1 (3%)
3	CAP	C	446	2	20,20,20	0.77	0	31,31,31	1.37	4 (12%)
3	CAP	D	446	2	20,20,20	0.73	0	31,31,31	1.15	3 (9%)
3	CAP	E	446	4	20,20,20	0.74	0	31,31,31	1.07	3 (9%)
3	CAP	F	446	2	20,20,20	0.76	0	31,31,31	0.99	1 (3%)
3	CAP	G	446	2	20,20,20	0.76	0	31,31,31	1.13	2 (6%)
3	CAP	H	446	2	20,20,20	0.75	0	31,31,31	1.30	4 (12%)
3	CAP	I	446	2	20,20,20	0.75	0	31,31,31	1.11	3 (9%)
3	CAP	J	446	4	20,20,20	0.79	0	31,31,31	0.87	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAP	A	446	2	-	0/29/29/29	0/0/0/0
3	CAP	B	446	2	-	0/29/29/29	0/0/0/0
3	CAP	C	446	2	-	0/29/29/29	0/0/0/0
3	CAP	D	446	2	-	0/29/29/29	0/0/0/0
3	CAP	E	446	4	-	0/29/29/29	0/0/0/0
3	CAP	F	446	2	-	0/29/29/29	0/0/0/0
3	CAP	G	446	2	-	0/29/29/29	0/0/0/0
3	CAP	H	446	2	-	0/29/29/29	0/0/0/0
3	CAP	I	446	2	-	0/29/29/29	0/0/0/0
3	CAP	J	446	4	-	0/29/29/29	0/0/0/0

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	446	CAP	O7-C-C2	3.44	121.08	113.58
3	H	446	CAP	O7-C-C2	3.40	120.98	113.58
3	C	446	CAP	C3-C2-C	-3.05	103.71	109.20
3	B	446	CAP	O7-C-C2	2.99	120.10	113.58
3	D	446	CAP	O7-C-C2	2.89	119.88	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	436/444 (98%)	-0.11	12 (2%)	50	62	17, 28, 49, 58	0
1	B	437/444 (98%)	0.00	19 (4%)	34	45	14, 26, 56, 62	0
1	C	437/444 (98%)	0.10	27 (6%)	20	29	16, 27, 60, 66	0
1	D	437/444 (98%)	0.11	18 (4%)	35	47	15, 26, 58, 85	0
1	E	432/444 (97%)	-0.10	12 (2%)	50	62	15, 25, 53, 70	0
1	F	437/444 (98%)	0.08	18 (4%)	35	47	17, 30, 57, 64	0
1	G	437/444 (98%)	-0.02	22 (5%)	28	39	13, 25, 52, 58	0
1	H	438/444 (98%)	0.12	34 (7%)	13	20	16, 28, 58, 61	0
1	I	437/444 (98%)	-0.17	15 (3%)	43	54	13, 24, 52, 70	0
1	J	434/444 (97%)	-0.03	20 (4%)	31	42	14, 25, 57, 74	0
All	All	4362/4440 (98%)	-0.00	197 (4%)	32	43	13, 27, 56, 85	0

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	425	ALA	7.6
1	C	421	LEU	7.4
1	G	434	ALA	7.2
1	D	421	LEU	7.1
1	E	441	VAL	6.8

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy

less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	KCX	D	189	12/13	0.21	1.51	21,22,24,25	0
1	KCX	B	189	12/13	0.18	1.22	18,20,21,22	0
1	KCX	A	189	12/13	0.17	1.21	20,23,24,24	0
1	KCX	F	189	12/13	0.17	0.96	23,25,27,27	0
1	KCX	H	189	12/13	0.15	0.80	20,21,25,26	0
1	KCX	C	189	12/13	0.16	0.41	21,22,26,28	0
1	KCX	G	189	12/13	0.13	0.24	16,19,20,20	0
1	KCX	J	189	12/13	0.16	-0.12	19,19,24,26	0
1	KCX	I	189	12/13	0.13	-0.15	19,21,25,25	0
1	KCX	E	189	12/13	0.12	-0.20	18,19,23,24	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	H	445	1/1	0.23	2.41	22,22,22,22	0
2	MG	C	445	1/1	0.25	2.40	23,23,23,23	0
3	CAP	C	446	21/21	0.21	0.82	23,34,37,39	0
3	CAP	J	446	21/21	0.20	0.78	20,28,40,40	0
2	MG	B	445	1/1	0.17	0.70	19,19,19,19	0
4	CA	J	445	1/1	0.19	0.57	27,27,27,27	0
3	CAP	H	446	21/21	0.17	0.36	24,35,37,39	0
3	CAP	E	446	21/21	0.16	0.17	16,27,37,38	0
2	MG	G	445	1/1	0.15	-0.11	22,22,22,22	0
3	CAP	B	446	21/21	0.15	-0.14	18,29,35,36	0
3	CAP	D	446	21/21	0.15	-0.15	18,28,31,32	0
3	CAP	G	446	21/21	0.14	-0.18	16,29,33,34	0
3	CAP	I	446	21/21	0.13	-0.41	15,25,27,28	0
3	CAP	F	446	21/21	0.15	-0.58	24,33,34,35	0
3	CAP	A	446	21/21	0.12	-0.93	21,30,31,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	E	445	1/1	0.12	-2.15	27,27,27,27	0
2	MG	D	445	1/1	0.14	-2.25	27,27,27,27	0
2	MG	A	445	1/1	0.09	-2.40	32,32,32,32	0
2	MG	I	445	1/1	0.09	-3.41	21,21,21,21	0
2	MG	F	445	1/1	0.04	-9.22	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.